EXOMOL ROVIBRATIONAL LINELIST FOR NaO

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Sodium oxide (NaO) is observed in airglows in the Earth's atmosphere and likely has astronomical importance. This study concerns the transitions with X $^2\Pi$ and and to the very low-lying ($T_0 < 2000$ cm^{-1}) A $^2\Sigma^+$ state. A line list consisting of energy levels, allowed transitions, Einstein coefficients, and a partition function are produced based on variational solution of the coupled rovibronic Schrödinger equations using program Duo[a]. Ab initio calculations which characterized the potential energy, spin-orbit, Λ-doubling and (transition) dipole moment curves were used as starting points to form the final model. Ab initio PECs were parameterized using Morse potentials and improved by least-squares fitting to experimental data on the rotational spectrum by Yamada et al [b] and the electronic spectrum by Joo et al [c]. A lack of data detailing the dissociation energies and vibrational structure of the X and A states prompts a request for further experimental study into the species which would allow further improvement of the model.

[a] S. Yurchenko, L. Lodi, J. Tennyson, A.V. Stolyarov, *Comput. Phys. Comm.*, 2016, **202**, 262-275

[b] C. Yamada, M. Fujitake, E. Hirota, *J. Chem. Phys*, 1989, **90**, 3033

[c] S. Joo, D.R. Worsnop, C.E. Kolb, S.K. Kim, D.R. Herschbach, *J. Phys. Chem.*, 1999, **103**, 3193-3199